

NA-ASC-500-07 Issue 2

January 2007

The View from HQ



Sitting in airports and planes is risky beyond the obvious dangers now in the news. Uninterrupted time to think may lead to new ideas. Instinct instructs us that when we hear Washington has some new ideas, the result must be bad. After all, ideas suggest change, which is inherently disruptive.

Today the notion of *predictivity* is on my mind as I am leaving the V&V 2007 meeting in Los Alamos. *Predictivity* is on my short list of overused, ill-defined words. Washington maintains a full lexicon of such words—a fair number of which find their way into common usage. Despite its ambiguities, the concept of *predictivity* spurs some thoughts regarding change in

the nuclear weapons complex.

The nuclear weapons enterprise, which I believe is still coasting on post cold-war momentum, is in need of re-evaluation. We face the increased "virtualization" of our world in decades to come. To prepare ourselves for the unforeseeable future, we will need to develop a virtual milieu that is conducive to exploration of ideas with sufficient integrity so we can respond when, and if, technological surprises arise. When sufficient technical data are unavailable, *predictivity* will become essential—our *sine qua non*.

The new ASC 2020 Roadmap emphasizes the need for *predictivity*. Emphasizing *predictivity* and technology as underpinnings, I would like to remove critical phenomenology from the simulation codes in three-year cycles. For us to embrace the need for *predictivity*, we will need to forego the old, tired rationale, "that's the way we always have done it."

The Thermonuclear Burn Initiative (TBI) illustrates my point. I initiated this just over a year ago, to provide a long-term, unconstrained intellectual environment with resources to allow researchers to step back and question traditional approaches to problems of great interest. Today, this initiative has become an exciting computational science leadership effort. If you are not acquainted with it, you should be.

We need more ideas along the lines of the TBI. I will continue to think strategically about such issues, at airports and other "quiet" places. I particularly welcome your thoughts and specific suggestions that have not yet been considered or tried to help us move forward.

Successful Completion of ASC Purple Integration Impresses Review Panel

The fiscal year 2007 Level 1 Milestone to provide a 100-teraFLOPs platform environment supporting the tri-laboratory Directed Stockpile Work and Campaign simulation requirements was met with flying colors, as determined by a nine-member review panel composed of representatives from academia, the Department of Defense, the Department of Energy, and the National Nuclear Security Administration (NNSA) tri-laboratory community.

The panel, chaired by Professor Paul Woodward, University of Minnesota, met at Lawrence Livermore National Laboratory to review the milestone on December 14 and 15, 2006. After the review, the panel declared in its initial report that the milestone had been successfully completed. A written panel report will be submitted to the Department of Energy for concurrence. Following are some selected comments from the panel's initial report:

- The panel was extremely impressed by the successful completion of the Purple integration, user support, and getting the system into use by the ASC community.
- End-to-end tri-lab user tests showed a high level of user satisfaction.
- The stability and reliability of the system are clearly very good.
- The quality of user support appears to be outstanding.
- The LLNL team deserves special accolades for accomplishing all this while at the same time bringing up the BlueGene/L system in the same building.
- The excellent team at LLNL did such a fine job of integrating the Purple system and making it available for productive use that the committee spent much of its deliberative time formulating suggestions for work that goes beyond the requirements of this Level 1 Milestone.

See the Livermore ASC Web site for more information about ASC Purple. [http://www.llnl.gov/asc/computing_resources/purple/]

2006 Gordon Bell Prizes Awarded to Lawrence Livermore's BlueGene/L Simulations

A large-scale electronic structure simulation of the heavy metal molybdenum conducted on the world's fastest supercomputer, BlueGene/L, earned a team led by a former and current Lawrence Livermore National Laboratory (LLNL) scientists the 2006 Gordon Bell Prize for "peak performance."



Livermore's BlueGene/L supercomputer, which was instrumental in winning two 2006 Gordon Bell prizes.

Three teams were selected from six finalists for Gordon Bell Prizes in two categories. A team from IBM's Thomas J. Watson Research Center also was awarded a "Special Achievement" Gordon Bell Prize for work on BlueGene/L, and a Japanese team earned a Gordon Bell peak performance honorable mention. The awards were announced at SC06 in Tampa, FL. This supercomputing conference is an international conference for high-performance computing, networking, storage, and analysis. Named for one of the founding fathers of supercomputing, the prestigious Gordon Bell Prize is awarded to innovators who advance high-performance computing.

Led by Francois Gygi, formerly of Lawrence Livermore and currently at UC Davis, LLNL's peak performance team includes IBM's TJ Watson Research Center, Carnegie Mellon University, and the Institute of Analysis and Scientific Computing at the Vienna University of Technology, Vienna, Austria. Their entry was titled "Large-Scale Structure Calculations of High-Z Metals on the BlueGene/L Platform."

Molybdenum, a high-Z or heavy metal, is of particular interest to scientists with the National Nuclear Security Administration's (NNSA) Stockpile Stewardship Program. NNSA scientists use simulation to better understand the effects of aging on nuclear materials. The team used Qbox, a first principles molecular dynamics (FPMD) code, to achieve simulations of unprecedented scale and detail.

Qbox demonstrates excellent parallel efficiency and peak performance. A sustained peak performance of 207.3 teraFLOPs was measured on 65,536 nodes, corresponding to 56.5 percent of the theoretical full machine peak using all 128k central processing units.

"Conducting predictive simulations of heavy metals, such as molybdenum, is a very challenging problem which requires a machine of BlueGene/L's capabilities," said Erik Draeger of Livermore's Center for Ap-

plied Scientific Computing. "It's a challenge because this code has to do many things very efficiently to accurately render a simulation. Heavy metals are very complex elements."

This kind of simulation is much larger than any previously feasible FPMD simulation. Such calculations open the way for accurate simulations of the properties of metals, including the calculation of melting temperatures, defect energies and defect migration processes, and the study of the effects of aging on the structural and electronic properties of heavy metals and materials subjected to extreme conditions. Understanding the properties of heavy metals is critical to the Stockpile Stewardship Program.

Los Alamos Completes First-of-Its-Kind Physics Code Assessment

A comprehensive verification and validation (V&V) assessment of a coupled-physics primary burn code was completed at Los Alamos National Laboratory (LANL) in September. The code evaluation entailed comparisons of simulation results with theory and data, as well as extensive spatial and temporal convergence analyses. Single-physics test problems included problems from the Tri-Laboratory Test Suite such as the Noh and Sedov problems for hydrodynamics and the Sood-Forster problems for neutronics. New test problems were developed for radiation transport. Integral-physics test problems included selected problems from the JOWOG 42 suite among others. Separate effects test validation efforts concentrated on various criticality experiments. Validation of integrated simulation capabilities focused on Nevada Test Site results for a specific, well-instrumented event.

As intended, the results of the V&V assessment spotlighted areas where the code produced excellent results and, more importantly, where improvements in the code and code usage were warranted. Code enhancement efforts were prioritized by extensive sensitivity analyses. Both single-variable and multivariable sensitivity analyses were performed. Sensitivities to both physical and numerical parameters were evaluated and compared. A high-value by-product of the assessment was developing recommendations for end users for using the code effectively.

Critical Level 1 Verification & Validation Milestone Completed

An external review panel convened at ASC headquarters on December 5, 2006, to review completion evidence for a FY06 Level 1 Milestone to "deliver advanced ASC physics and engineering simulation capabilities to support the W76 and W80 LEP/certification." Sandia's contribution to the milestone consisted of (1) validating fire model predictions of heat flux to a weapon; (2) quantifying weapon safety margins and uncertainty in fire environments; (3) determining adequacy of arming, fuzing & firing (AF&F) assembly response predictions in a hostile blast environment. A Level 2 Milestone was completed in each of these areas. The panel concurred that the milestone had been successfully completed.

The panel summarized the significance of the milestone completion as follows: "For the first time, a quantification of margins and uncertainty (QMU) analysis of a critical nuclear safety stronglink/weaklink thermal race in an abnormal thermal environment (hydrocarbon fuel fire) can now be performed. Historically, evidence was provided with limited test data and frequently supported with subjective engineering assessments. We now have a viable QMU process that will provide additional quantifiable evidence for weapon system qualification and the ability to identify margins and uncertainties against nuclear safety requirements.

The system-level shock response to hostile endo-atmospheric blast is an environment that cannot be simulated with high fidelity in a ground test. Therefore, to support system design and qualification, a structural dynamics model was developed and validated using blast-tube test data from an instrumented reentry body and (AF&F) unit. This model successfully calculated the necessary structural responses to generate the subsystem and component-level mechanical environment specifications. The modeling provided the design engineers with higher fidelity specifications for this hostile environment than had been supplied on previous reentry systems. It was recognized that efforts need to continue to model and simulate the complete tactical environment for hostile endo-atmospheric blast."

Verification Analyses Method Developed

Los Alamos scientists Trevor Tippets, Frank Timmes, Jim Kamm, and Jerry Brock recently completed an initial exploration of a new method that performs verification analyses on complex multi-physics problems where an exact solution is unknown. The new method uses an optimization technique to estimate the exact solution in tandem with a self-consistent convergence rate. Unlike previous efforts, their new

method allows for oscillatory convergence, which is observed to occur near shock fronts or material discontinuities. This step in technology is key to bridging the gap between analytical test problems and highly complex applications.

The main plot compares the estimated exact solution for the density produced by the new method (purple) with the analytical solution (red) for a blast wave solution on a 1D uniform mesh. The inset plot details the convergence rate of the estimated exact solution.

Award Winning Data Analysis Toolkit Released

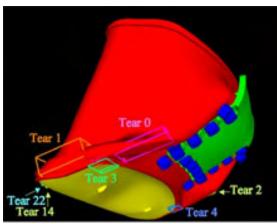
It is difficult for computers to understand a simple thing like a tear in a sheet of metal. Standard data visualization techniques do not do the job, either, as material failures like tears may happen anywhere in a simulation. With massive datasets, the problem becomes much worse. There could be thousands of features that an analyst is interested in. How can we harness computation to help with this problem?

To address these needs, Sandia has developed "FCLib," a data analysis toolkit constructed to meet the needs of data discovery in large-scale, spatio-temporal data. Funded via the ASC Pre- and Post-Processing Environment, FCLib is a C library toolkit of building blocks that can be used to assemble analyses for rich, quantitative, and convenient post-processing.

FCLib "characterizations" (codes that automate extraction of information from ASC simulation data) have supported a number of ASC analyses. In particular, FCLib analysis and staff were among the winners of the Gold Level Sandia President's Quality Award bestowed on the "Validation, Verification, and Quantified Margins and Uncertainties for Modeling and Simulation of W80-3 Handling Drops" project.

An example of FCLib post-processing analysis is the detection and characterization of tears. The figure on the left, below, illustrates the appearance of a tear in a weapon drop experiment. Even in close-up, it can be difficult to detect, and even harder to quantify. The figure on the right is the result of an analysis built with the FCLib code. Not only does the characterization place labeled bounding boxes to aid visual inspection, but it also extracts and records quantitative measures of the severity of the tear, such as total volume, length, and maximum width of the tear.





FCLib is open source software available under a Berkeley Software Distribution (BSD)-like license. It is available at http://fclib.ca.sandia.gov.

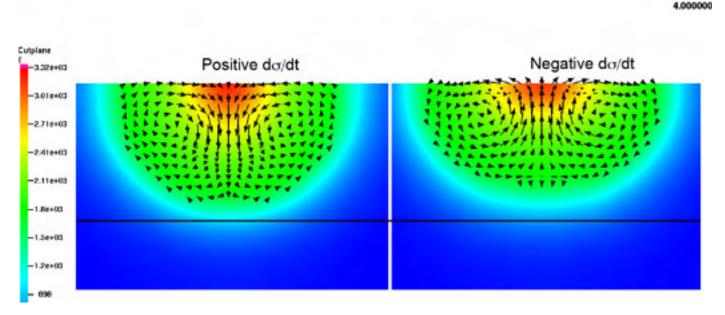
Truchas Software Applications Extended within Complex

As part of the ASC Engineering Verification and Validation (V&V) project, the Los Alamos casting simulation software Truchas has been assessed for extending its application to other problems such as welding within the DOE Nuclear Weapons Complex.

Truchas is a 3D casting simulation code, a product of the ASC-funded Telluride project. Truchas simulates the entire casting process: flow of molten alloy, heat transfer, solidification of alloy, induced stresses, etc.

Two QuickTime movies generated from Truchas simulations show 3-D animation sequences of weld pool development in two cases of laser spot welding. The color scale is temperature (Kelvin), and the number at the top right corner indicates time (t) (in seconds). At t=0, a laser beam is activated to heat and melt stainless steel at a spot on its top surface for a duration of 4 ms. After the beam is turned off, the weld

pool begins to cool and completely re-solidifies at 6.6 ms. Black arrows indicate velocity vectors, which also mark the presence of liquid (i.e., define the weld pool region). The two movies illustrate opposite signs of the parameter do/dT—the coefficient of change of surface tension with respect to temperature. The simulations show that for a positive coefficient, the flow is downward in the center, giving rise to a deeper weld penetration, as compared with the case for a negative coefficient (see also figure, below). While the simulation is 3D, the 2-D representation shown in these movies represent a slice of the calculation results at the center of the simulation. This study employed experimental data from the LANL Welding and Joining Team and the Sandia Joining and Coating Department, in collaboration with Penn State University researchers for the validation problems.



Comparison of the two simulations at equivalent times. Black horizontal line is artificially inserted to assist in ascertaining deeper weld penetration in the simulation, at left (positive coefficient).

Xyce Electrical Modeling and Simulation to Support Weapons Qualification

In FY07, the Xyce circuit modeling application was used to generate simulation results in support of weapon components qualification efforts. To provide the greatest impact to qualification, the simulations focused on performance issues surrounding critical electronic subsystems. The circuit model has been enhanced to simulate relevant realistic scenarios by adding parasitic elements and initial conditions. The simulations provide additional qualification evidence by confirming design margins, giving access to circuit response measures not available during tests, and allowing for simulation of realistic hostile radiation scenarios that cannot be tested. The simulation results show good agreement with available test data, and validation efforts are under way in FY07, including several novel validation experimental activities.

The goal of the Xyce team is to provide distinctive capabilities in the area of circuit simulation through large-scale parallel computing, predictive transient-radiation device-models and combined (x/gamma ray, neutron, temperature) effects to weapons designers at Sandia. This suite of attributes is absolutely unique and has been specifically developed to support the unique mission-space of Sandia's electrical design and qualification community. The inclusion of these results in qualification documentation represents a major accomplishment towards that goal.

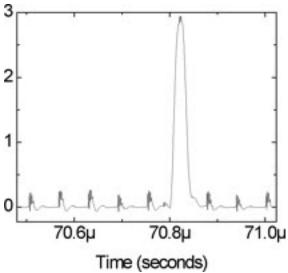


Figure 1. Simulation showing total photocurrent created in a critical electronic subsystem as a result of an ionizing radiation event. This total photocurrent response cannot be measured during a test.

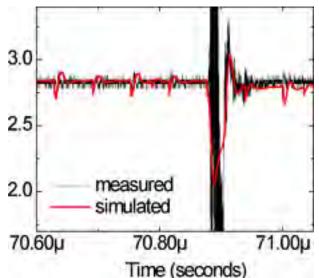
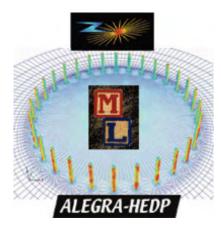
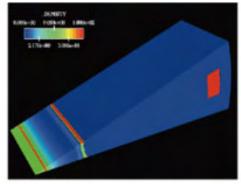


Figure 2. Ionizing radiation simulation showing good agreement with measured data for a critical circuit response measure and confirming design margins.

An Improved H-curl Algebraic Multigrid Solver for Z-pinch Simulations





The liner implodes to the axis without instability: An important step in Z-pinch simulations!

Sandia's ML solver team [http://software.sandia.gov/trilinos/packages/ml/] has resolved an extremely challenging technical issue associated with the solution of singular and ill-conditioned H(curl) matrices for ALEGRA-HEDP Z-pinch simulations.

A parallel H(curl) algebraic multigrid solver was adapted to address conductivity variations ranging over eight orders of magnitude as well as to allow for regions of zero conductivity (or void regions). These extreme conditions require special care in how operators are coarsened and how errors are smoothed within the solver. Simulations involving large conductivity variations and significant mesh stretching are needed for highly accurate simulations that avoid spurious magnetic Rayleigh-Taylor instabilities in the overall solution of a liner implosion problem.

As a result of efforts in both linear solvers and in the proper numerical representation of the underlying physics, a simulation recently and for the first time ran through the peak of the main power pulse without exhibiting magnetic Rayleigh Taylor instability induced by background noise. The intended symmetric magnetic field solution was produced. This achievement is an important step toward modeling and simulation of Z-pinch phenomena.

Subsequent simulations will allow analysts to determine the effects of slots and gaps on system behavior, which will be relevant in determining how to redesign the load to eliminate undesirable features in experiments on the Z-machine. The solver enhancements have been incorporated in the Trilinos Library [http://software.sandia.gov/trilinos/] and represent a substantial advance in the solvability of H(curl) systems arising during Z-pinch simulations. A completely new H(curl) algebraic multigrid solver is also under development. This new solver is based on an exact discrete algebraic reformulation of the H(curl) problem and takes advantage of a discrete Hodge decomposition. Numerical experiments indicate that this future H(curl) solver will be even less sensitive to the dramatic material variations common in Z-pinch experiments.

Load Balancing Work Receives Best Paper Award

Researchers from Sandia and Ohio State University were awarded the Best Paper award in the Algorithms track of the 2007 International Parallel and Distributed Processing Symposium (IPDPS). The paper, *Dynamic Load Balancing for Adaptive Scientific Computations via Hypergraph Repartitioning*, presents a novel algorithm for redistributing data in adaptive parallel simulations. Authors are Erik Boman, Karen Devine, Robert Heaphy, and Lee Ann Fisk Riesen of Sandia, and Umit Catalyurek and Doruk Bozdag of Ohio State University.

As an adaptive simulation's computational requirements change, the algorithm rebalances processor workloads while keeping interprocessor communication costs and data redistribution costs low. The new method exploits the robust and accurate hypergraph partitioning model to reduce average total communication costs by roughly 20% compared to traditional graph repartitioning methods. The algorithm will be released this winter in the Zoltan Parallel Data Management Toolkit, open-source software available at http://www.cs.sandia.gov/Zoltan.

IPDS is a highly competitive international conference (sponsored by IEEE) covering all aspects of parallel computation, including algorithms, applications, architectures, and system software. The award-winning paper was judged best of the 419 submissions to the Algorithms track. The award will be presented March 28, 2007, in Long Beach, CA.

Sixth Annual Nuclear Weapons Engineering Analysis Conference (NWEAC)

Sandia National Laboratories hosted the sixth annual Nuclear Weapons Engineering Analysis Conference at Monterey, CA, on September 5-8, 2006. Approximately 70 engineering analysts from Sandia, Los Alamos, Lawrence Livermore, Kansas City Plant, and Y-12 met to discuss their respective nuclear weapons engineering simulations.

Topical areas covered at this classified conference included (1) assessments of confidence in engineering models and their usefulness for specific applications and assessment of weapon performance based on these models, (2) examples of quantification of margins and uncertainty (QMU) applications, (3) analysis for safety, transportation, and manufacturing, and (4) analysis challenges/requirements for certifying new designs.

Bob Stevens from Los Alamos received a best paper award for his talk entitled "Comparison of Some W76-1 Hostile Environments and Their Ground Test Surrogates." Attendees agreed that NWEAC continues to be the best forum for the nuclear weapons engineering community for discussing their issues on computational simulation. The seventh annual NWEAC is scheduled for September 4-6, 2007 in Monterey.

Los Alamos Hosts Tri-Lab V&V Workshop

Beginning Tuesday, January 9, 2007, and ending with a half-day on Friday, January 12, the ASC Verification and Validation (V&V) Workshop was held at Los Alamos, with participation limited by invitation to tri-lab V&V managers. After an introductory talk by Dimitri Kusnezov, the workshop began with the following topical areas: Primary Validation, Thermonuclear Application Validation, Engineering V&V, Code and Calculation Verification, Uncertainty Quantification, Tri-Lab Test Suites, Data Analysis, Software Quality Engineering (SQE), and others.

The workshop's objectives were as follows:

Technical exchange on V&V as required by the ASC engineering and physics-simulation community;

- Discussion on the FY07 Level 2 Milestone: tri-lab study of verification methods;
- Engagement with ASC Alliance technical staff.

BlueGene/L Is Still the Fastest Computer in the World

The 28th TOP500 List was released in Tampa, FL, during SuperComputing 2006. On the new list, the BlueGene/L system retains the No. 1 spot with a Linpack performance of 280.6 teraFLOPSs.

[http://www.top500.org/lists/2006/11]

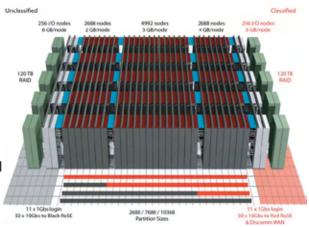
Red Storm Ranks No. 2 on Top 500 List



When the Top500 supercomputer list (http://www.top500.org/lists/2006/11) was announced at Supercomputing 2006, Red Storm placed second overall, and first among the general-purpose high-end computer systems that are useful for a broad range of the ASC portfolio of engineering and scientific analysis codes. Its Linpack performance is 101.4 teraFLOPs.

Between August and October 2006, Sandia and Cray successfully up-

graded Red Storm by integrating a fifth row to increase the number of compute nodes from 10,368 to 12,960. The single core 2.0 GHz AMD Opteron processors were exchanged for dual core 2.4 GHz processors, and the initial SeaStar 1.2 was exchanged for SeaStar 2.1 NIC/Router interconnect chips—a change that effectively doubled the bandwidth performance of the interconnect sub-system. Sandia modified the Red Storm lightweight kernel operating system to provide a simple method for using the second core on each compute node for Message Passing Interface (MPI) applications. These combined hardware and software changes increased the measured Linpack performance from 36.19 teraFLOPs to 101.4 teraFLOPs.



ASC Booth at SC06 Conference Demonstrates NNSA's Achievements in High-Performance Computing



ASC Booth, 2006

With a theme of "Predictive Simulation with Confidence," the ASC booth at SC06 once again presented ASC's many achievements at the International Conference on High-Performance Computing, Networking, Data Storage, and Analysis. Sponsored by the Association for Computing Machinery (ACM) and the Institute of Electrical and Electronics Engineers (IEEE) Computer Society, this year's conference was held in Tampa, FL, from November 11 to 17th.

Led by Los Alamos this year, the booth hosted ASC participants from

the each laboratory who served on conference committees, presented at technical conference sessions, and set up the booth. Booth

participants had a full schedule of presentations and demonstrations. The booth featured a 3D theater contributed by Los Alamos and a kiosk demonstrating the work of the Lawrence Livermore Center for Applied Scientific Computing (CASC).

ASC (formerly ASCI) has been exhibiting its lab-developed technologies at Supercomputing since 1996. The first tri-lab booth was set up at the conference in Pittsburgh.



ASC1 Booth, 1996

IBM and BlueGene/L Continue Domination of HPCC Competition at SC06

For the second year, IBM and BlueGene/L dominated the High-Performance Computing Challenge (HPCC) competition at the annual SuperComputing Conference (SC06). The DOE/NNSA/Lawrence Livermore National Laboratory team, using IBM's BlueGene/L system, once again swept all four Class 1 (best performance) benchmark awards, proving BlueGene/L's ability to solve a wide range of computational problems. The four Class 2 productivity awards were split among MIT, IBM, The MathWorks, and the Russian People Friendship University.

The Class 1 HPCC benchmarks—High-Performance Linpack, RandomAccess, fast Fourier transform, and STREAM-system—are focused on raw performance. The first place winner of each benchmark was awarded a \$500 prize. The HPCC awards were presented at the HPCC award booth at SC06, and the prizes were sponsored by *HPCWire* magazine. Tom Spelce of Lawrence Livermore accepted the awards on behalf of the team.

Background

In 2003, the DARPA's High Productivity Computing Systems released the HPCC suite. It examines the performance of HPC architectures using kernels with various memory access patterns of well-known computational kernels. Consequently, HPCC results bound the performance of real applications as a function of memory access characteristics and define performance boundaries of HPC architectures. The suite was intended to augment the TOP500 list, and the results are publicly available for 6 out of 10 of the world's fastest computers. Implementations exist in most of the major high-end programming languages and environments, accompanied by countless optimization efforts.

Sandia's ASC Russia Program Hosts Russian Collaborators



A group of Russian scientists from the Russian Academy of Sciences' Institute of Problems in Mechanical Engineering in St. Petersburg and its Institute of High Energy Densities in Moscow attended the first of two ASC-supported annual project reviews of the Russia Science and Technology Program.

Hosted by Sandia at its Livermore site from October 16-19, the eight visiting scientists and engineers from both institutes met with their Sandia collaborators E.P.(Tony) Chen (manager of Mechanics of Materials, Dept. 8776) and John Aidun (manager of Multiscale Dynamic Materials Modeling, Dept. 1435) and their respective staff. Technical exchanges included reporting on current projects: Performance and Reliability Modeling of MEMS (microelectromechanical systems), Atomistic Study of Phonon Generation and Evolution by Laser Excitation, and Application of Non-Equilibrium

Molecular Dynamics (NMED) Simulation Methods. Additional technical exchanges explored directions for continued or new projects in the areas of atomistic materials simulation for improved understanding of a diverse range of material behaviors from solid mechanics fracture to non-equilibrium plasmas. All projects focus on the development and application of high-performance computing methods to advance predictive science and engineering capabilities, consistent with the goals of the ASC Program.

The success of these technical exchanges has far exceeded one of the original goals of improving the communications between technical workers in the two countries. New ideas proposed are now leading to additional research projects that enhance ongoing work being performed at Sandia.

TSF Team Honored with DOE Project Management Award

The Terascale Simulation Facility (TSF) [http://www.llnl.gov/asc/tsf/] Project at Lawrence Livermore National Lab has recently won the DOE Secretary's Project Management Award of Achievement.

The Project Management Awards are presented annually to three teams that demonstrate outstanding performance based on overall management and successful completion of a project.



Anita Zenger, the Lab's TSF Project Manager, accepted the award on behalf of the TSF team during a DOE conference for contractor project managers and federal project directors in Alexandria, VA, in mid-November.

The TSF is a 253,000-square-foot facility that houses world-class super-computers and more than 250 staff. The facility designers had to carefully consider and balance safety and efficiency, and the need for flexibility to address changing computing technology. Innovations in the TSF's design include heating and cooling for demanding computer systems, advanced computer cooling capabilities, highest achievable clear space and effec-

tive use of natural lighting for offices. The building was completed in late 2004, eight months ahead of schedule and \$1.2 million under budget.

"I am proud that the team produced a computing asset for the Lab that is second to none," said Barbara Atkinson, the TSF team's Computation Directorate management liaison. "[The TSF] positions our lab well for the future."

The first Lawrence Livermore Laboratory building dedicated to computing to be constructed in 20 years, the TSF will become the home for next-generation supercomputers. Photos and text documenting the pre-construction site view and artists's renderings, the groundbreaking, month-by-month construction progress, and the ribbon-cutting



ceremony are available in the TSF Construction Scrapbook. [http://www.llnl.gov/asc/tsf/tsf_scrapbook/]

Sandia Wins Award for Red Storm Video

A video showcasing the Red Storm Supercomputer at Sandia National Laboratories has received a Finalist Award in the prestigious 2007 New York Festivals International Film and Video Competition in the Mathematics and Computer Science Category. The video, "Red Storm Visualization Tour," was produced by a Sandia team to provide an option to physical tours of the supercomputer. Actual scientific simulations performed on Red Storm are interspersed with creative animations and dramatic flyovers of the computer to make the experience better than a walk-through tour in many ways.

The New York Festivals seeks to recognize "The World's Best Work" in informational, educational, and industrial film productions and corporate video. The competition also covers short film, feature-length film, and home videos. Now approaching its 50th anniversary, the Film & Video Awards sees entries from over 30 countries around the world. Entries are judged by panels of international award winning creatives who are recognized as leaders in their respective fields.

Sandia team members involved in the production of the video include John Zepper, John Noe, Constantine Pavlakos, Bob Ballance, Regina Valenzuela, Jon Goldman, Lisa Ice, Patricia Crossno, and David Karelitz.

Awards will be presented at a ceremony in New York City on February 2, 2007. [http://www.newyorkfestivals.com]

Transitions

Rathkopf Named Associate Program Leader for Computational Physics; Graziani Named Associate B Division Leader for Computational Physics

To continue and expand collaboration in code development between Lawrence Livermore National Laboratory's A and B Programs—the two departments responsible for design and analysis of nuclear warheads—Livermore Physicist **James A. Rathkopf** recently was named Associate A and B Program Leader for Computational Physics within the Defense and Nuclear Technologies Program. In this role, Rathkopf will continue solely the leadership of the ASC Integrated Codes sub-program, a position he shared in recent years.



James A. Rathkopf

Also, Livermore Physicist **Frank R. Graziani** was selected for the dual role of Associate B Division Leader for Computational Physics and the Deputy Associate B Program Leader for Computational Physics. Graziani will work with Rathkopf directing the effort and budget for B Program's code-development. Rathkopf, Graziani, and **Dennis W. Hewett**, A Program's Deputy Associate Program Leader for Computational Physics, will coordinate computational physics activities with various programs across Livermore Laboratory, with particular emphasis



Frank R. Graziani



Dennis W. Hewett

given to managing the Livermore ASC Integrated Codes sub-program and coordinating code collaborations. Formerly, Graziani supported legacy and ASC codes, and he was the B Program Verification and Validation lead.

Thorp Named ASC CCSE Program Manager

John Hopson and Stephen Lee are pleased to announce the selection of **John Thorp** as the permanent ASC CCSE Program Manager. John will report to Stephen Lee, the CCS Division Leader and also, programmatically, to John Hopson, the ASC Program Director. John Thorp will manage scope, schedule, and budget for the Computer Systems and Software Environment program element of the ASC Program. John has been acting in this role since earlier this spring. His appointment is effective November 13, 2006.

ASC Salutes

Editor's note: Each quarter, the ASC Program will feature the outstanding contributions of one of its numerous tri-lab scientists, engineers, and administrators. This month, we proudly present Hank Childs.



Barely thirty years old, Computer Scientist **Henry (Hank) R. Childs** has already won an R&D 100 award and is now part of a team that will bridge high-performance computing visualization efforts between the Department of Energy's National Nuclear Security Administration and Office of Science.

Childs is one of the computer scientists responsible for the Lawrence Livermore National Laboratory (LLNL) program VisIt, a data analysis and visualization tool that recently won an R&D 100 award from the trade journal *R&D Magazine* for being among the top 100 industrial innovations worldwide for 2005. VisIt was developed for Advanced Simulation and Computing (ASC) scientists to study massive data sets. "I interact daily with ana-

lysts and code developers to determine what analysis techniques are needed to study their simulations," said Childs. "We then use VisIt to deliver these metrics to

our user community. VisIt provides an infrastructure for processing petascale data and is now relatively mature, so it allows us to deploy our efforts quickly and efficiently. Our goal was to go beyond pretty pictures; it was to create a product with techniques for reducing the complexity of the data in a way that allowed our scientists to be confident in their analysis and not be concerned that important data was somehow being lost." VisIt's capabilities span data exploration, code debugging, quantitative analysis, movie making, and comparative analysis.

VisIt will be one of the primary deployment vehicles for VACET (the Visualization and Analytics Center for Enabling Technologies), a SciDAC (Scientific Discovery through Advanced Computing) center tasked with providing peta-scale visualization and analysis solutions to Office of Science customers. "I think there is strong commonality between the efforts of this center and our ASC efforts, starting primarily with peta-scale visualization and analysis, but also including specific techniques like topological characterization, comparative visualization, statistics-based visualization,

The Office of Science's Sci-DAC (Scientific Discovery through Advanced Computing) Program awarded \$2.2M per year for five years to VACET (Visualization and Analytics Center for Enabling Technologies), a multi-institutional center (Livermore, Lawrence Berkeley, and Oak Ridge National Laboratories, UC Davis, and the University of Utah), to meet production visualization needs for Office of Science customers; Livermore's VisIt software will be the primary deployment vehicle.

and high-dimension data, such as energy groups. It was that commonality that made the partnering so attractive," said Childs. Despite taking on these new responsibilities, Childs will remain part-time with ASC, pursuing verification and validation work on shape characterization.

Childs began his career with Lawrence Livermore after receiving his Bachelor of Science degree in both math and computer science from the University of California at Davis. After graduating, Childs took a few years off school to marry, start his family, and begin his work at Livermore. With two young children at home, he started the PhD program in April 2000, attending school evenings and weekends, and finished his graduate studies at the end of 2006.

For more information: http://www.llnl.gov/visit http://www.vacet.org

ASC Web Site

http://www.sandia.gov/NNSA/ASC/

Newsletter Points of Contact

Send submittals to:

Vin Lopresti—Los Alamos National Laboratory vcl@lanl.gov
Andrea Baron—Lawrence Livermore National Laboratory baron1@llnl.gov
Reeta Garber—Sandia National Laboratories ragarbe@sandia.gov

Who's Who

ASC Program Managers—Headquarters

Director, Office of Advanced Simulation and Computing, NA-114

<u>Dimitri Kusnezov</u>—Dimitri.Kusnezov@nnsa.doe.gov

Ken Alvin—kfalvin@sandia.gov
April Commodore—april.commodore@nnsa.doe.gov
Njema Frazier—njema.frazier@nnsa.doe.gov
Thuc Hoang—thuc.hoang@nnsa.doe.gov
Sander Lee—sander.lee@nnsa.doe.gov
Ed Lewis—edgar.lewis@nnsa.doe.gov
Bob Meisner—bob.meisner@nnsa.doe.gov
Denise Peoples—denise.peoples@nnsa.doe.gov
Erich Rummel—erich.rummel@nnsa.doe.gov

ASC Program Managers—Labs

Los Alamos National Laboratory

<u>John Hopson</u>—jhopson@lanl.gov

<u>Cheryl Wampler</u>—clw@lanl.gov

<u>Ralph Nelson, Deputy Program Director (acting)</u>—ran@lanl.gov

Lawrence Livermore National Laboratory

<u>Michel McCoy</u>—mccoy2@llnl.gov

<u>Lynn Kissel, Deputy Program Manager</u>—kissel1@llnl.gov

Sandia National Laboratories
Art Hale—alhale@sandia.gov
Robert Thomas, Enabling Capabilities—rkthoma@sandia.gov
Paul Yarrington, Simulation Applications—pyarrin@sandia.gov



SAND 2007-0482W

Developed and maintained by Sandia National Laboratories for NA.114